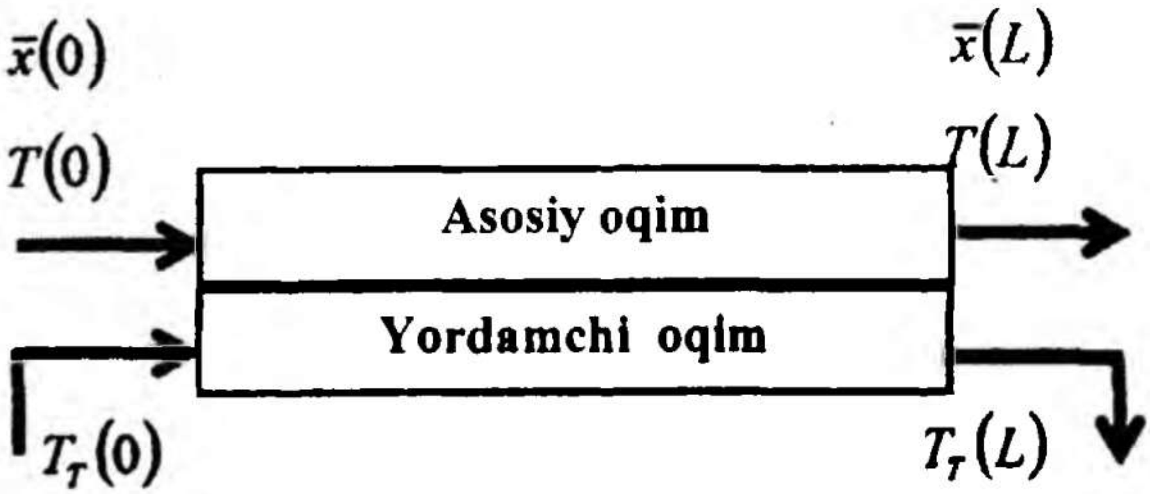
bo'lgan shartlarda uning tekshiruv (baholash) hisoblash algoritmining blok - sxemasini tuzish.

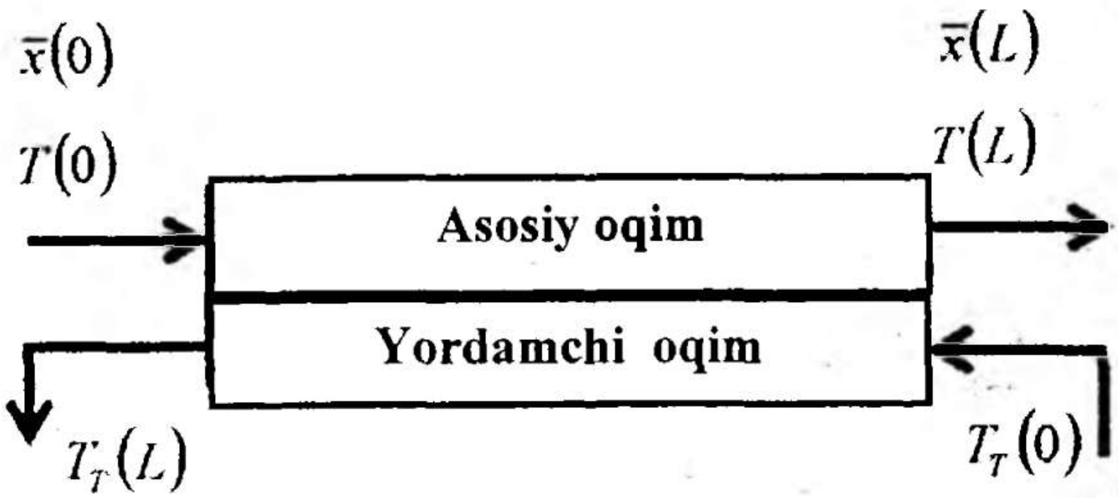
5.1.5 Quvurli reaktorlarni hisoblash va algoritmlashtirish

5.1.5.1. Politropik reaktorning statsionar rejimi

a) Issiqlik tashuvchi to'g'ri oqim rejimida harakatlanadi(Koshi masalasi va boshlang'ich shartli masala).



b) Issiqlik tashuvchi teskari oqim rejimida harakatlanadi (Chegaraviy masala).



Asosiy qo'yimlar:

– mikrokinetika: reaksiya

$$2A \xrightarrow{k_1} 3B \xrightarrow{k_2} C$$

$$(-\Delta H_1) \quad (-\Delta H_2)$$

– oqimlar harakati ideal o‘rin almashishning gidrodinamik modellari bilan keltiriladi;

– bosqichlarning issiqlik samaralari haroratlarga bog‘liq emas;

– asosiy oqim va qobiqdagi oqimlar o‘rtasidagi issiqlik almashuvida faqat issiqlik uzatish ishtirok etadi;

– issiqlik uzatish koeffitsiyenti = const.

Jarayonning mikrokinetikasi

$$2A \xrightarrow{k_1} 3B \xrightarrow{k_2} C$$

Aniqlanadi:

$g_A^R,\ g_B^R,\ g_C^R,\ \Delta q^R,$

$$\begin{bmatrix} g_A^R \\ g_B^R \\ g_C^R \end{bmatrix} = \begin{bmatrix} -2 & 0 \\ 3 & -3 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} k_1 x_A^2 \\ k_2 x_B^3 \end{bmatrix} = \begin{bmatrix} -2k_1 x_A^2 \\ 3k_1 x_A^2 + 3k_2 x_B^3 \\ k_2 x_B^3 \end{bmatrix}$$

$$\bar{g}^R = \bar{\bar{\alpha}} \cdot \bar{r}$$

$$g_A^R = -2 \cdot r_1$$

$$g_B^R = 3 \cdot r_1 - 3 \cdot r_2$$

$$rang(\bar{\bar{a}}) = 2$$

2 ta hal qiluvchi A va V komponentalarni tanlaymiz

$$g_C^R = -\frac{1}{2} g_A^R - \frac{1}{3} g_B^R$$

Muhim bo‘lmagan S komponenta uchun stexiometrik munosabat:

$$x_C = x_C^{(0)} - \frac{1}{2}\left(x_A - x_A^{(0)}\right) - \frac{1}{3}\left(x_B - x_B^{(0)}\right)$$

$$\Delta q^R = \sum_{j=1}^{2} \left|\alpha_{p_j}\right| \left(-\Delta H_{p_j}\right) \cdot r_j = 3\left(\Delta H_{B1}\right) \cdot r_1 + 1\left(-\Delta H_{C2}\right) \cdot r_2$$

Jarayonning matematik tavsifi (to‘g‘ri oqim).

1.1) $x_A \dfrac{dv}{d\ell} + v \dfrac{dx_A}{d\ell} = \dfrac{V_R}{L} g_A^R \Rightarrow \dfrac{dx_A}{d\ell} = \dfrac{V_R}{vL} g_A^R - \dfrac{x_A}{v} \dfrac{dv}{d\ell}$

1.2) $\dfrac{dx_B}{d\ell} = \dfrac{V_R}{L} g_B^R - \dfrac{x_B}{v} \dfrac{dv}{d\ell}$

1.3) $x_C = x_C^{(0)} - \frac{1}{2}\left(x_A - x_A^{(0)}\right) - \frac{1}{3}\left(x_B - x_B^{(0)}\right)$

2.1) $g_A^R = -2 \cdot r_1$

2.2) $g_B^R = 3 \cdot r_1 - 3 \cdot r_2$

2.3) $g_C^R = r_2$

3.1) $r_1 = k_1 x_A^2$

3.2) $r_2 = k_2 x_B^3$

4.1) $k_1 = A_1 \exp(-E_1/RT)$

4.2) $k_2 = A_2 \exp(-E_2/RT)$

5) $\frac{dv}{d\ell} = \frac{V_R}{L}\left(g_A^R + g_B^R + g_C^R\right)$

6)
$$\frac{d(vT)}{d\ell} = \frac{V_R}{C_p L}\Delta q^R + \frac{F_T}{C_p L}\Delta q^T \Rightarrow$$
$$\Rightarrow \frac{dT}{d\ell} = \frac{V_R}{vC_p L}\Delta q^R + \frac{F_T}{vC_p L}\Delta q^T - \frac{T}{v}\cdot\frac{dv}{dl}$$

7) $\Delta q^R = 3(-\Delta H_{B1})r_1 + (-\Delta H_{C1})r_2$

8) $\Delta q^T = K^T\left(T_T - T\right)$

9) $C_p = C_{p_A}^{ind} x_A + C_{p_B}^{ind} x_B + C_{p_C}^{ind} x_C$

10.1) $C_{p_A}^{ind} = a_A + b_A T + c_A T^2 + d_A T^3$

10.2) $C_{p_B}^{ind} = a_B + b_B T + c_B T^2 + d_B T^3$

10.3) $C_{p_C}^{ind} = a_C + b_C T + c_C T^2 + d_C T^3$

Issiqlik tashuvchilarning oqimlari uchun tenglama:

11) $\frac{dT_T}{d\ell} = \frac{F^T}{C_{P_T} L v_T}\left(-\Delta q^T\right)$

n+3 differensial tenglama.

Boshlang'ich shart:

(1.1') $x_A(0) = x_A^{(0)}$

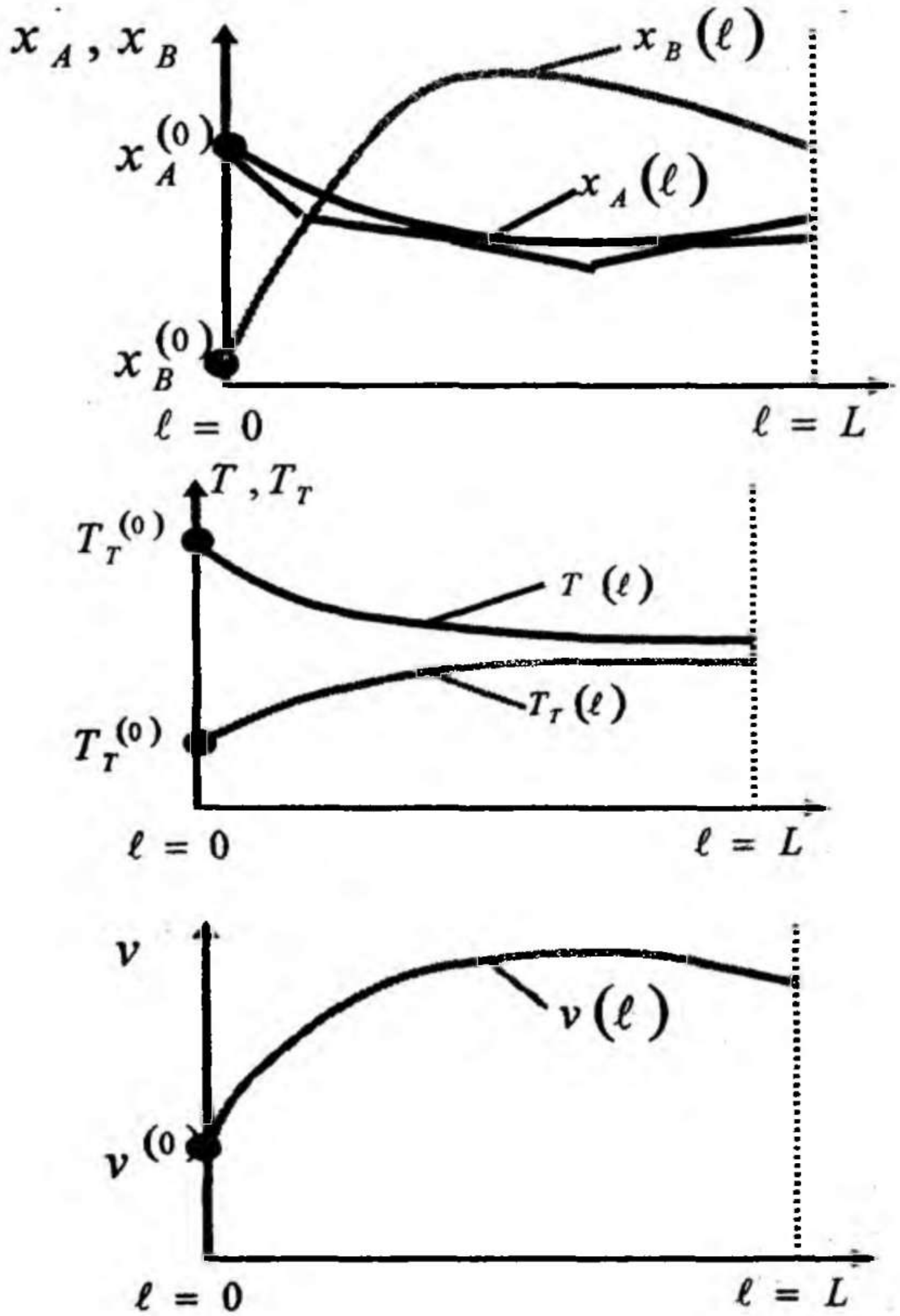
(1.2') $x_B(0) = x_B^{(0)}$

(5') $v(0) = v^{(0)}$

(6') $T(0) = T^{(0)}$

$$(11')\ T_T(0) = T_T^{(0)}$$

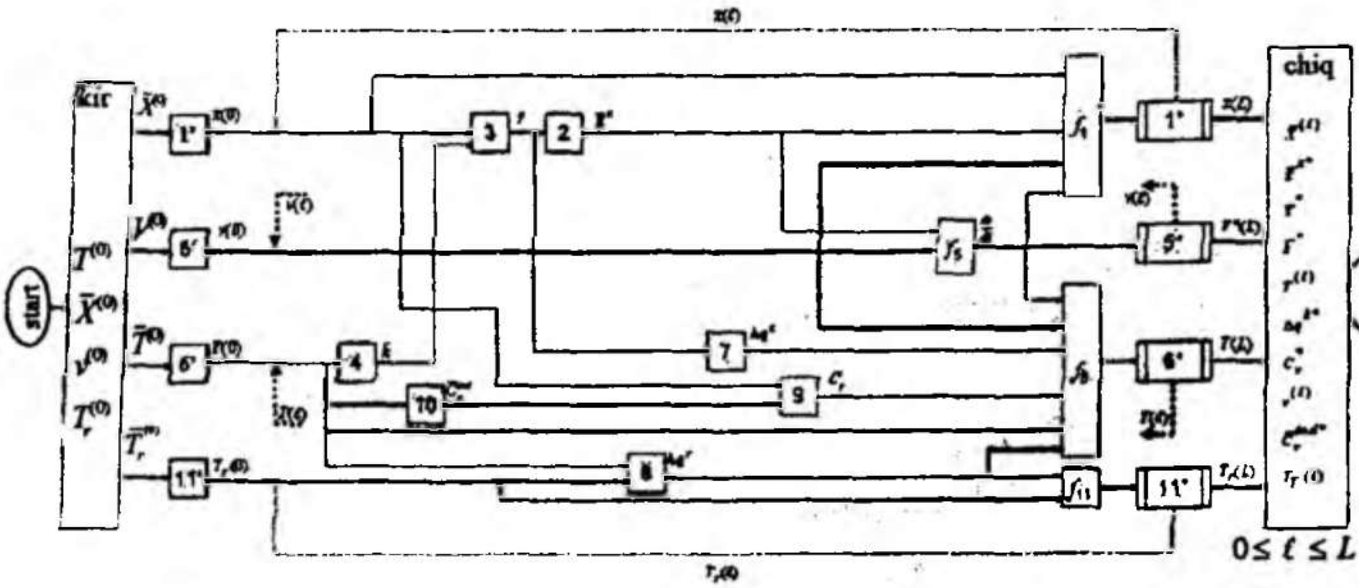
Kompyutyerda xususiy yechimni aniqlash uchun Koshi masalasi yoki boshlang'ich shartli masala yechiladi – «o'rin almashish – urin almashish» issiqlik almashish apparatiga qarang (to'g'ri oqim).



Axborot matritsasi (to‘g‘ri oqim)

n \ p	$x_A(0)$	$x_A(L)$	$x_B(0)$	$x_B(L)$	$x_C(0)$	$x_C(L)$	$\bar{g}^R_{(n)}$	$\bar{r}_{(m)}$	$\bar{k}_{(m)}$	$T(0)$	$T(L)$	Δq^T	Δq^R	C_p	$v(0)$	$v(L)$	f_5	$C^{bof}_{p(n)}$	$T_r(0)$	$T_r(L)$	N^o
$\bar{1}_{(n)}$	●	◆	●	◆	●	◆	●								●		●				14
$\bar{2}_{(n)}$							◆	●													8
$\bar{3}_{(n)}$	●		●		●			◆	●												7
$\bar{4}_{(n)}$									◆	●											5
5*															●	◆	●				13
5*.1							●								●		◆				12
6*										●	◆	●	●	●	●		●				15
7								●					◆								10
8										●		◆							●		9
9	●		●		●									◆				●			11
$\overline{10}_{(t)}$										●								◆			6
11*												●		●					●	◆	16
$\bar{1}_{(n)}$	◆		◆		◆																1
5′															◆						2
6′										◆											3
11′																			◆		4

Hisoblash algoritmining blok-sxemasi (to‘g‘ri oqim)



Jarayonning matematik tavsifi (teskari oqim).

Ideal o‘rin almashish modelining komponentli balansi:

1.1) $x_A \dfrac{dv}{d\ell} + v\dfrac{dx_A}{d\ell} = \dfrac{V_R}{L} g_A^R \Rightarrow \dfrac{dx_A}{d\ell} = \dfrac{V_R}{vL} g_A^R - \dfrac{x_A}{v}\dfrac{dv}{d\ell}$

1.2) $\dfrac{dx_B}{d\ell} = \dfrac{V_R}{L} g_B^R - \dfrac{x_B}{v}\dfrac{dv}{d\ell}$

1.3) $x_C = x_C^{(0)} - \frac{1}{2}\left(x_A - x_A^{(0)}\right) - \frac{1}{3}\left(x_B - x_B^{(0)}\right)$

2.1) $g_A^R = -2 \cdot r_1$

2.2) $g_B^R = 3 \cdot r_1 - 3 \cdot r_2$

2.3) $g_C^R = r_2$

3.1) $r_1 = k_1 x_A^2$

3.2) $r_2 = k_2 x_B^3$

4.1) $k_1 = A_1 \exp(-E_1/RT)$

4.2) $k_2 = A_2 \exp(-E_2/RT)$

5) $$\frac{dv}{d\ell} = \frac{V_R}{L}\left(g_A^R + g_B^R + g_C^R\right)$$

6) $$\frac{d(vT)}{d\ell} = \frac{V_R}{C_p L}\Delta q^R + \frac{F_T}{C_p L}\Delta q^T \Rightarrow$$
$$\Rightarrow \frac{dT}{d\ell} = \frac{V_R}{vC_p L}\Delta q^R + \frac{F_T}{vC_p L}\Delta q^T - \frac{T}{v}\cdot\frac{dv}{d\ell}$$

7) $\Delta q^R = 3(-\Delta H_{B1})r_1 + (-\Delta H_{C1})r_2$

8) $\Delta q^T = K^T\left(T_T - T\right)$

9) $C_p = C_{p_A}^{ind} x_A + C_{p_B}^{ind} x_B + C_{p_C}^{ind} x_C$

10.1) $C_{p_A}^{ind} = a_A + b_A T + c_A T^2 + d_A T^3$

10.2) $C_{p_B}^{ind} = a_B + b_B T + c_B T^2 + d_B T^3$

10.3) $C_{p_C}^{ind} = a_C + b_C T + c_C T^2 + d_C T^3$

Issiqlik tashuvchilarning oqimi uchun tenglama:

11) $$\frac{dT_T}{d\ell} = \frac{F^T}{C_{P_T} L v_T}\left(-\Delta q^T\right)$$

n+3 differensial tenglama, to‘g‘ri oqim bilan solishtirilganda faqat (11) tenglama o‘zgaradi.

Boshlang‘ich shartlar tizimi:

(1.1') $x_A(0) = x_A^{(0)}$

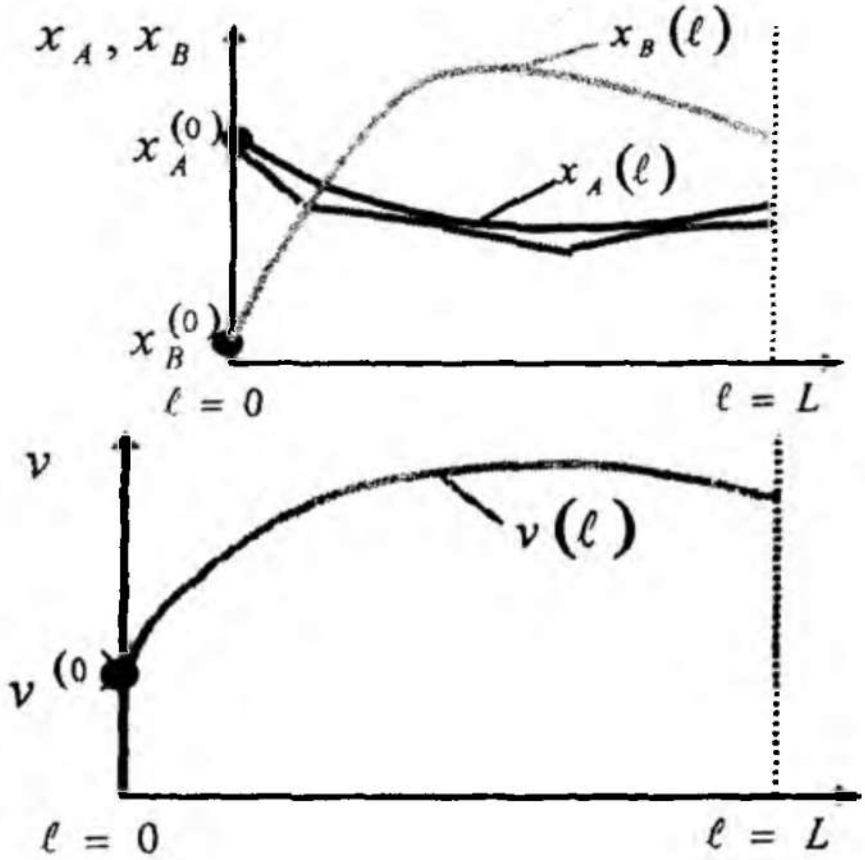
(1.2') $x_B(0) = x_B^{(0)}$

(5') $v(0) = v^{(0)}$

(6') $T(0) = T^{(0)}$

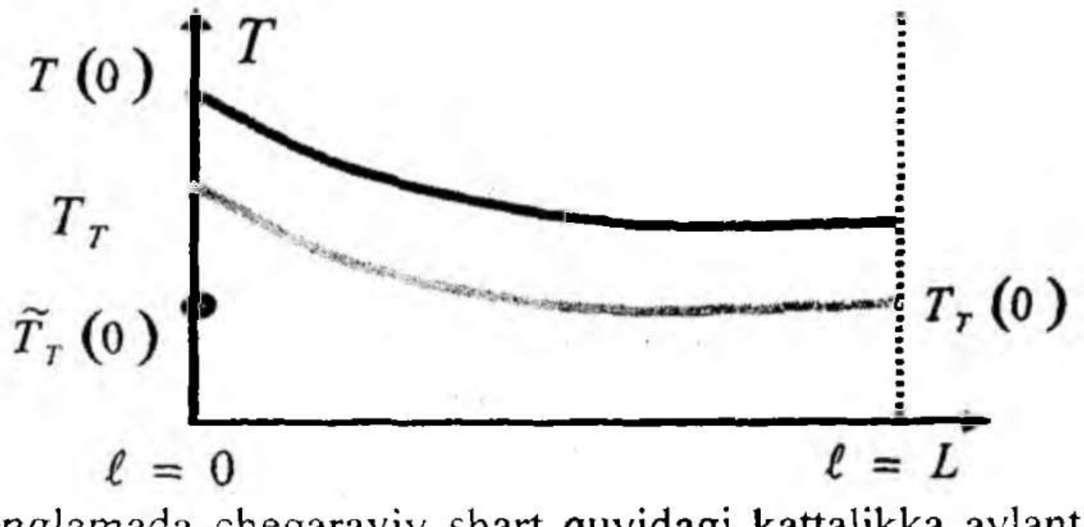
(11') $T_T(0)=T_T^{(0)}$

Kompyuterda xususiy yechimni aniqlash uchun chegara shartli chegaraviy masala yechiladi – «o‘rin almashish – o‘rin almashish» issiqlik apparatiga qarang (teskari oqim).



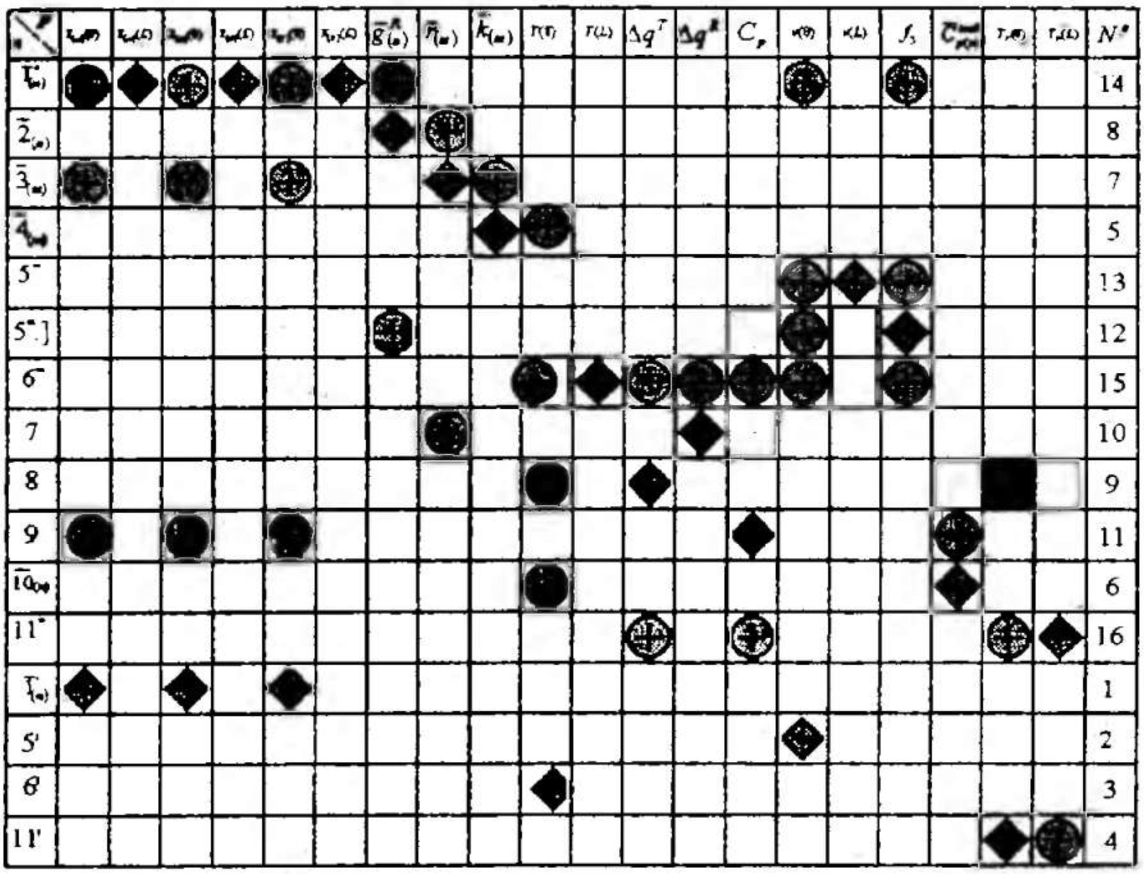
Boshlang‘ich yaqinlashish:

$\tilde{T}_T(0)$

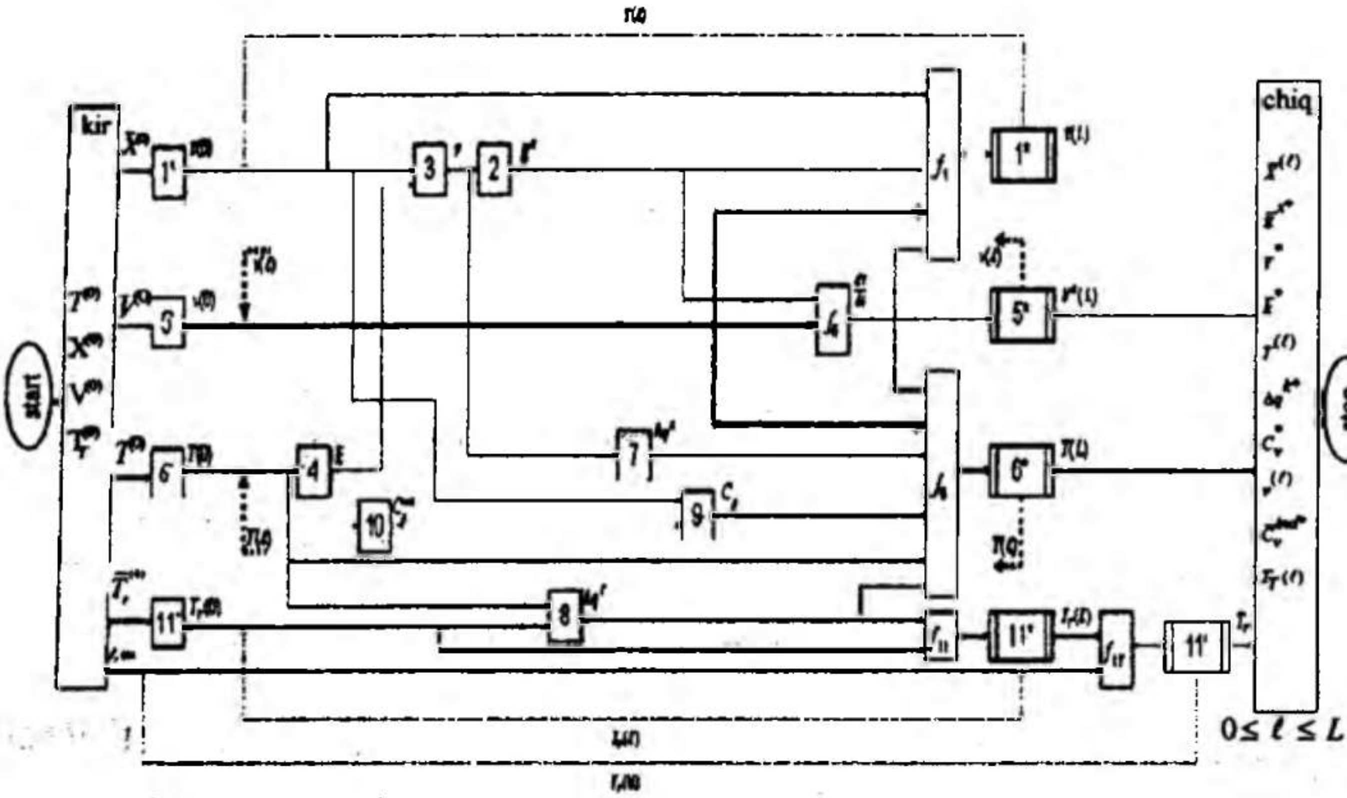


Tenglamada chegaraviy shart quyidagi kattalikka aylantiriladi: $\tilde{T}_T(0)$, ya’ni kirishga issiqlik tashuvchi haroratining kattaliklari.

Axborot matritsasi (teskari oqim)



Hisoblash algoritmining blok-sxemasi (teskari oqim)



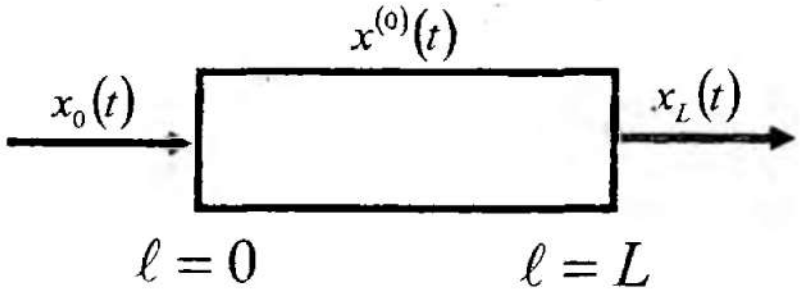
$T_T(\ell = 0) \Rightarrow T_T(0)$

11') tenglamaning yechimi:

$T_T(0)*$

$f_{1'} = T_T(L)\{T_T(0)\} - T_T^{(0)} = 0$

5.1.5.2. Nostatsionar rejimdagi quvurli reaktorlar



$A \xrightarrow{k} P$

Asosiy qo'yimlar:

Izotermik rejim;

Bir parametrli diffuziyali model.

Matematik tavsifning tenglamasi:

$$\frac{V^R}{L}\frac{\partial x}{\partial t} = \frac{DV^R}{L}\frac{\partial^2 x}{\partial \ell^2} - v\frac{\partial x}{\partial \ell} + G^R_{A(\ell)}$$

$$x = [A];\ S = \frac{V^R}{L};\ G^R_{A(\ell)} = \frac{V^R}{L} g_A = -kx,\ V = S \cdot W$$

$$1)\ \ \frac{\partial x}{\partial t} = D\frac{\partial^2 x}{\partial \ell^2} - W\frac{\partial x}{\partial \ell} - kx$$

1) tenglama ikki mustaqil o'zgaruvchi t va ℓ ga ega parabolik tipdagi ikkinchi tartibli xususiy hosilali differensial tenglama hisoblanadi va agar oqim uchun bir parametrli diffuziyali model qabul qilingan bo'lsa, yagona oddiy reaksiya oqib o'tuvchi reaktorning nostatsionar rejimini tavsiflaydi.

Topish lozim:

$x = x(t, \ell)$

$t^{(0)} \le t \le t^{(k)}$

$0 \le \ell \le L$

Boshlang'ich shart:

1') $x(t^{(0)}, \ell) = x^{(0)}(\ell),\ \ 0 \le \ell \le L$

Chegaraviy shart:

$$1'')\ \begin{cases} x(t,0)=x_0(t) \\ x(t,L)=x_L(t) \end{cases} \quad t^{(0)}\le t\le t^{(k)}$$

Xususiy hosilalarda differensial tenglamalar tizimi (XHDTT) ni yechish uchun hosilasi ma'lum $\left[t^{(0)},t^{(k)}\right]$ va/yoki $[0,\ L]$ intervaldagi chekli – farqli shaklda namoyon bo'luvchi diskretlashtirish usulidan foydalanish mumkin, natijada 1') va 1'') chegara shartli 1) tenglama chekli tenglamalar tizimi (CHTT) dagi va/yoki oddiy differensial tenglamalar tizimi (ODTT) ga aylanib qoladi.

Bu tenglamalar uchun diskretlashtirishning uchta variantdan foydalanish mumkin:

1) ℓ mustaqil o'zgaruvchi bo'yicha:

$$\frac{\partial x}{\partial \ell}\cong\frac{x_{i+1}-x_i}{\Delta\ell}$$

$$i=1,..n-1$$

Natijada t mustaqil o'zgaruvchili 1 – tartibli oddiy differensial tenglamalar tizimi olinadi.

2) Mustaqil t o'zgaruvchi bo'yicha:

$$\frac{\partial x}{\partial t}\cong\frac{x_{j+1}-x_j}{\Delta\ell}$$

$$j=1,...m-1$$

Natijada ℓ mustaqil o'zgaruvchili 2 – tartibli oddiy differensial tenglamalar tizimi olinadi.

3) ℓ va t mustaqil o'zgaruvchilar bo'yicha:

$$\frac{\partial x}{\partial \ell}\cong\frac{x_{i+1}-x_i}{\Delta\ell}$$

$$i=1,..n-1$$

$$\frac{\partial x}{\partial t}\cong\frac{x_{j+1}-x_j}{\Delta\ell}$$

$$j=1,...m-1$$

Natijada chekli tenglamalar tizimi olinadi.

Mustaqil o'zgaruvchi bo'yicha diskretlashtirishning 1 - variantini batafsil ko'rib chiqamiz:

$0\le\ell\le L$ da hosilalarning chekli - ayirmali keltirilishi quyidagi ko'rinishga ega: